CENTER FOR COMPUTATIONAL ENGINEERING

DIABLO: Scalable, Implicit Multi-Mechanics for Engineering Simulation

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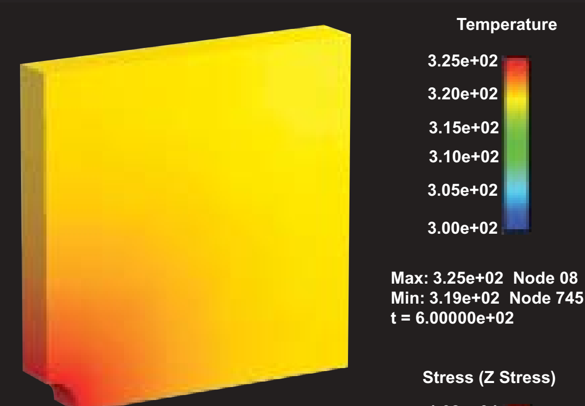
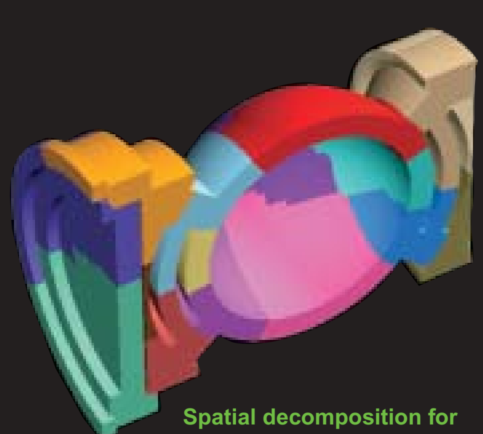
PURPOSE: The Diablo code project, which is funded under the NNSA's Advanced Simulation and Computation (ASC) Program, is creating a capability for engineering simulation using implicit methodologies on massively parallel computers. In this context, "implicit" means numerical formulations that avoid the limitations of small, stable time steps associated with explicit formulations but at the cost of solving coupled linear systems of equations. This ability to use relatively large time steps makes implicit techniques preferred for the simulation of statics, quasi-static, and low-frequency dynamics. Thus Diablo is viewed as a complement to our ParaDyn code for explicit, nonlinear solid mechanics. Paradyn is already utilized for Directed Stockpile Work both at LLNL and LANL.

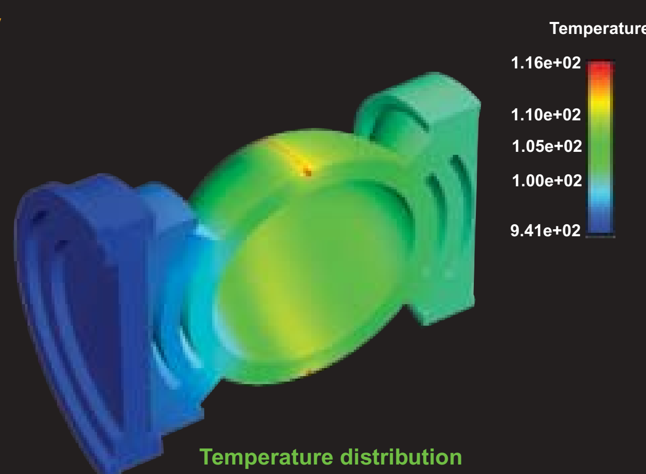
GOALS: Designed from the outset to simulate problems involving multiple physical phenomena, Diablo represents a new software architecture for the Methods Development Group. The example below shows the thermomechanical response of an assembly held with rigid axial constrains. Diablo is implemented with Fortran object-based data structures, which make it easier to add new functionalities. As an example, a capability for modeling surface chemical kinetics has been prototyped. The image at right illustrates a coupon sample's temperature response due to metal hydriding chemistry at the surface of a postulated defect.



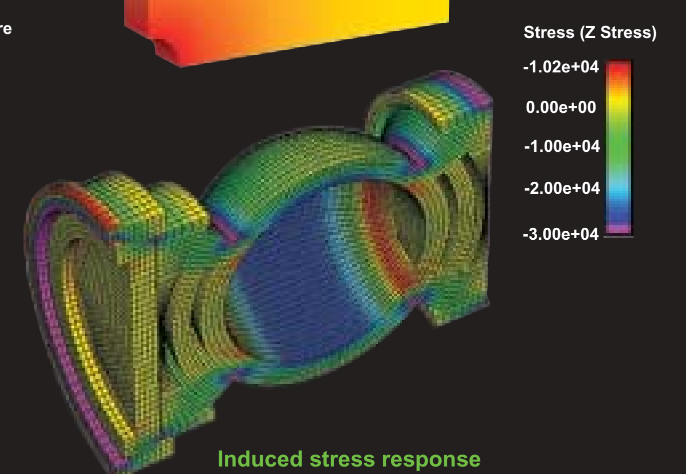
Modal Analysis Correlation Experiment Subassembly



Spatial decomposition for parallel processing



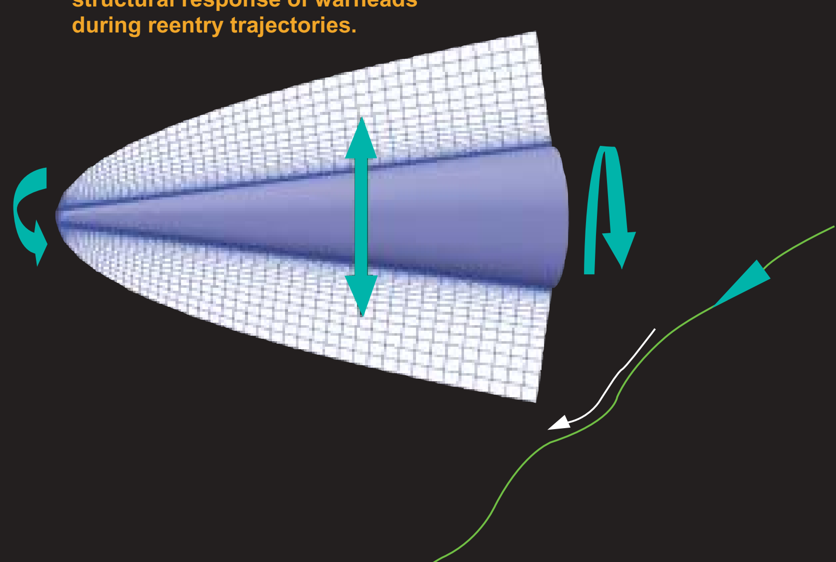
Temperature distribution from equatorial heat flux



Induced stress response due to end restraints

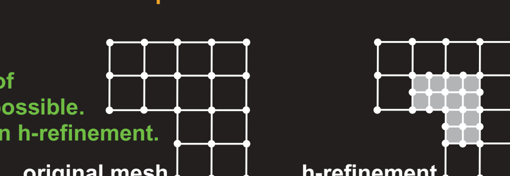
SUPPORTING RESEARCH: The flexibility of Diablo permits it to serve as a test bed for research and development of numerical methodologies with a direct path to a production capability. Two LDRD-funded projects in Mechanical Engineering are currently leveraging the ASC investment in Diablo. More broadly, because of the dependence of implicit simulation on efficient linear equation solving, Diablo is leveraging the ASC investment in solver libraries as made available through the Finite Element Interface API.

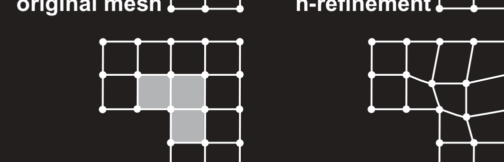
An LDRD project on hypersonic computational fluid dynamics (CFD) for meshes in noninertial frames is building a key component that will eventually aid in the transient simulation of the aero, thermal, and structural response of warheads during reentry trajectories.

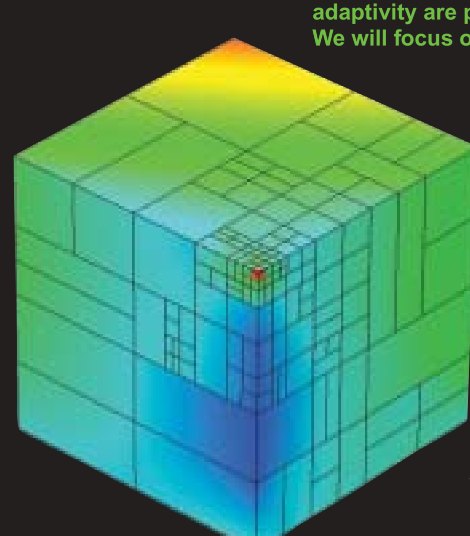


An LDRD project on adaptive mesh refinement will implement basic algorithms and investigate proposed error estimators in the context of nonlinear solid mechanics problems of interest to Engineering.

Multiple types of adaptivity are possible. We will focus on h-refinement.







A simple example with six levels of h-refinement.

Diablo
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